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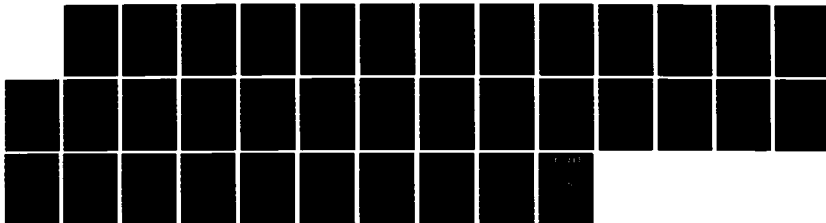
EXAMINATION OF A METHOD FOR PREDICTING THE PROPERTIES
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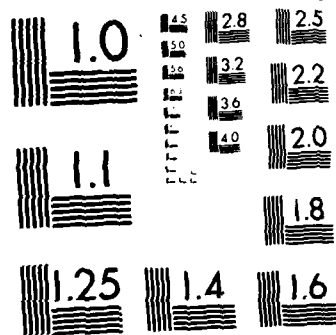
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MELBOURNE, VICTORIA

REPORT

MRL-R-960

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**EXAMINATION OF A METHOD FOR PREDICTING THE
PROPERTIES OF RAILGUN PLASMAS**

V. Kowalenko

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MATERIALS RESEARCH LABORATORIES**

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Basic studies of railguns require knowledge of the properties of plasmas. This report examines the work of Dr P. Kovitya who has developed two computer programs for predicting the thermochemical functions and transport coefficients of partially and fully-ionized gases in chemical equilibrium. Kovitya's work is based on extending the use of existing NASA codes from the temperature range of 300 to 5000 K to temperatures up to 30,000 K. In making these extensions, Kovitya has neglected the effect of screened Coulomb interactions on the ionization potentials of the various species comprising the ionised gas. This may produce significantly different numerical results for temperatures above 20,000 K. A detailed discussion of Kovitya's work is presented in this paper and the areas that require further consideration for the work to be applicable to a railgun plasma are highlighted.

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SECURITY CLASSIFICATION OF THIS PAGE

UNCLASSIFIED

DOCUMENT CONTROL DATA SHEET

REPORT NO. MRL-R-960	AR NO. AR-004-322	REPORT SECURITY CLASSIFICATION Unclassified
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TITLE

Examination of a method for predicting the properties of
railgun plasmas

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REPORT DATE

April, 1985

TASK NO.

DST 82/212

SPONSOR

DSTO

CLASSIFICATION/LIMITATION REVIEW DATE

April, 1988

CLASSIFICATION/RELEASE AUTHORITY

Superintendent, MRL
Physics Division

SECONDARY DISTRIBUTION

Approved for Public Release

ANNOUNCEMENT

Announcement of this report is unlimited

KEYWORDS

Plasma Diagnostics
Railgun Accelerators

COSATI GROUPS

2009

1906

ABSTRACT

Basic studies of railguns require knowledge of the properties of plasmas. This report examines the work of Dr P. Kovitya who has developed two computer programs for predicting the thermochemical functions and transport coefficients of partially and fully-ionized gases in chemical equilibrium. Kovitya's work is based on extending the use of existing NASA codes from the temperature range of 300 to 5000 K to temperatures up to 30,000 K. In making these extensions, Kovitya has neglected the effect of screened Coulomb interactions on the ionization potentials of the various species comprising the ionised gas. This may produce significantly different numerical results for temperatures above 20,000 K. A detailed discussion of Kovitya's work is presented in this paper and the areas that require further consideration for the work to be applicable to a railgun plasma are highlighted.

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SYMBOLS

a	speed of sound, m/s
a_i	polynomial coefficients used in equation (2)
\underline{B}	magnetic field of induction, W/m ²
b	impact parameter, m
C_p^o	heat capacity at constant pressure for standard state, J/(g-mole)(K)
c_p	specific heat at constant pressure, J/(g)(K) or cal/(g)(K)
C_p	specific heat at constant pressure, J/(g)(k) or cal/(g)(k)
D_j	correction term to account for screened Coulomb interactions for each species, j, (g-mole) ⁻¹ j
E	relative energy of colliding particles, J
e	electronic charge, $\sim 1.6 \times 10^{-19}$ C
g_i	degeneracy factor of the i-th excited state, dimensionless
$H(T)^o$	enthalpy for the standard state, J/g-mole
h	enthalpy, cal/g
j	current density, C/m ²
k	Boltzmann's constant, 1.381×10^{-23} J/K
l, s	integers used in specifying higher orders of Chapman-Euskog theory
M	molecular weight g/g-mole
m_e	electron mass, 9.11×10^{-31} kg
N_j	the number of particles of species j, dimensionless
n_j	g-moles of species j per g of mixture, (g-mole) _j /g
P	pressure, atm
$\underline{Q}^{(l)}(E)$	a quantity defined by equation (5), m ²
$Q_{ij}^{(l,s)}$	collision cross-section for species i colliding with species j, m ²
q^{00}, q^{01}, q^{11}	cross-section related expressions used to determine electrical conductivity, m ²

R	universal gas constant, 8314.3 J/(kg-mole)(K) or 1.9872 cal/(g-mol)(K)
r	separation distance between colliding particles, m
r_o	the solution to equation (7), m
$S(T)^o$	entropy for the standard state, J/(kg-mole)(K)
s	entropy, cal/(g)(K)
T	temperature, K
$V(r)$	interaction potential, J
x_e	mole fraction for electrons, dimensionless
x_j	mole fraction species j , dimensionless
Z	average charge number squared, dimensionless
γ	ratio of the heat capacity at constant pressure to that at constant volume, dimensionless
γ_{sp}	a function of \bar{Z} given by equation (13), dimensionless
ϵ	force constant appearing in equation (10), J
ϵ_i	energy of the i -th excited state, J
ϵ_o	permittivity of free space, $8.85 \times 10^{-2} \text{ C}^2/(\text{Nm}^2)$
η	viscosity, poise
θ	deflection angle between colliding particles, radians
λ	thermal conductivity of an ionised gas, J/(cm)(sec)(K)
λ_e	electron collision translation thermal conductivity, J/(cm)(sec)(K)
λ_{frozen}	thermal conductivity of the non-reacting part of the ionised gas, J/(cm)(sec)(K)
λ_{int}	thermal conductivity due to internal energy modes, J/(cm)(sec)(K)
$\lambda_{monatomic}$	thermal conductivity of the translational energy contribution for a single species, J/(cm)(sec)(K)
$\lambda_{reaction}$	thermal conductivity due to chemical reactions, J/(cm)(sec)(K)
μ_j	chemical potential of species j , J/(g-mole) $_j$
ρ	density, g/cm ³
ρ_D	Debye radius, m

σ	force constant appearing in equation (10), m
$[\sigma]_2$	electrical conductivity, S/cm
$\pi_{ij}^{(l,s)}$	collision cross-section for species i colliding with species j, m ²
ϕ	Gibb's free energy, J

C O N T E N T S

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EXAMINATION OF A METHOD FOR PREDICTING THE
PROPERTIES OF RAILGUN PLASMAS

1. INTRODUCTION

In his study of ablation-dominated arcs, which are found in fuses, lightning arrestors and circuit breakers, Kovitya [1] has used the expression 'material function' to denote the two types or classes of properties of most interest when studying plasma mixtures. These distinct types are: firstly, thermodynamic properties, which include such physical properties as the density, specific heat, enthalpy, heat capacity, molecular weight and speed of sound, and secondly transport properties, which include the electrical conductivity and the coefficients of viscosity and thermal conductivity. Many of the thermodynamic properties have not been considered to be particularly relevant in previous studies [2,3,4] of the plasma armature in electromagnetic railguns. Of the transport properties, the physical quantity of primary interest to railgun workers is the electrical conductivity. The remaining two transport properties have not been considered to be important in previous studies of the plasma in a railgun.

The electrical conductivity is of vital interest because it can be used to determine the potential difference across the plasma armature during a railgun firing. It is believed that the potential difference across the plasma should approach the voltage observed at the muzzle of the railgun. So far the plasma codes [2,3,4] for the railgun have failed to predict the muzzle voltage accurately. This suggests that the estimates for the electrical conductivity provided by these codes may be questionable or, alternatively, that plasma boundary effects may be much more significant than previously thought. In any case, Kovitya's code represents a different approach to determining the electrical conductivity of an arc or a plasma and may therefore give some indication of the accuracy of the estimates for the electrical conductivity used by the authors of the railgun codes.

2. BACKGROUND

In their analyses of railgun plasmas Thio [2], Batteh and Powell [3,4] have considered thermal conduction and viscosity effects to be negligible. Batteh and Powell [3] have shown that for a predominantly second-ionised plasma at a temperature T of 5.6×10^4 K with an electron number density n_e of 10^{26} particles/m³, and an assumed mean free path of about 10^{-4} m, the coefficient of radiation heat conduction is a factor of 15 times greater than the coefficient of thermal conductivity. This result led Batteh and Powell to conclude that radiation is substantially more important than thermal conduction. Because of this conclusion the solution of the energy conservation equation from the equations of magnetohydrodynamics is greatly simplified. However, the conditions just described for the plasma armature in an electromagnetic launcher (EML), or railgun, represent calculated values from the one-dimensional arc dynamics code developed by Batteh and Powell and hence they might not really represent the actual conditions of the plasma armature when more than one dimension is considered. It is believed [4] that the actual plasma is substantially cooler, which may mean that all the other properties associated with the plasma may change appreciably. The overall result would cast some doubt on Batteh and Powell's conclusion that thermal conduction is negligible.

Viscosity has not been discussed by Batteh and Powell. On the other hand Thio [2] shows how the momentum conservation equation from the equations of magnetohydrodynamics is affected by the inclusion of viscosity effects. However after introducing the equation he, also, assumes that viscosity effects are negligible and therefore puts the kinematic coefficient of viscosity equal to zero, thereby simplifying the momentum conservation equation considerably. These authors have therefore assumed that the viscosity-based force term appearing in the equation is negligible in comparison to the Lorentz-based ($\mathbf{j} \times \mathbf{B}$) force term for railgun plasmas since in these plasmas both the current density and magnetic field are large. The results provided by Kovitya [1] indicate that even for a non-magnetised plasma the viscosity drops significantly when the temperature is increased for a constant pressure or when the pressure is decreased for a constant (but fairly high) temperature. The situations just described mean that viscosity effects become less important as the degree of ionisation increases. Thus since railgun plasmas are considered to be highly ionised plasmas then viscosity effects may justifiably be considered as unimportant.

3. THERMODYNAMIC PROPERTIES

Before the thermodynamic properties of an ionised gas can be evaluated, the thermochemical functions of each component or species comprising the ionised gas must be found. The thermochemical functions referred to by Kovitya are the heat capacity at constant pressure for species j in the standard state, denoted by $(C_p(T))^{\circ}_j$, the enthalpy for species j at constant temperature in the standard state, denoted by $(H^{\circ}(T))^{\circ}_j$, and the entropy for species j at constant temperature in the standard state, denoted

by $(S(T)^0)$. In addition to requiring the thermochemical properties to calculate the thermodynamic properties, the compositions of each of the species j in terms of the number of moles are required.

The computer program used by Kovitya to calculate the compositions of the various species comprising an ionised gas is a NASA program written by Gordon and McBride [5]. For this program to be applicable to an ionised gas, the system must be in chemical equilibrium. Whether a railgun plasma is in chemical equilibrium or not is open to conjecture. Preliminary spectroscopic and metallurgic observations of the railgun used in experiments at MRL [6] have indicated that the initial plasma, which consists mainly of ionised aluminium from the metal foil fuse is continuously losing aluminium and replacing it with copper and other impurity ions derived principally from the rails throughout the firing. This inability of the magnetic field to completely confine the plasma behind the projectile in a railgun means that the concentrations of the various species comprising the plasma armature are changing during a firing and that the plasma is not strictly in chemical equilibrium.

According to Gordon and McBride [7], their method is only valid for temperatures between 300 and 5000 K, the range of applicability being limited by the validity of the ideal gas equation of state. Although this code is a separate program, it becomes one of the many subroutines within Kovitya's code and is called subroutine MAIN.

Because Kovitya is also interested in the fully ionised limit he has extended the range of applicability of the Gordon and McBride computer code to temperatures up to 30,000 K. This is justified only if the effect of screened Coulomb interactions can reasonably be neglected when calculating the chemical potential of each species. These interactions arise in a plasma because electrical charges of one sign tend to have, on an average, an excess of charge of the opposite size in their neighbourhood. This is commonly referred to as a charge cloud and is a result of the Coulomb interaction [7]. As a result of this plasma polarisation, a certain energy is released when an electron-ion pair is produced because each particle is somewhat attracted by the charges already present in the plasma. Thus the ionisation energies of each of the species are reduced from the values corresponding to their values when in isolation by an amount that depends on the charges of the particles, the plasma density and temperature.

Since the ionisation energies of free atoms or ions require corrections to account for the energy released on immersing an electron-ion pair in a plasma, this implies that bound states whose energies are between the reduced and uncorrected ionisation energies now become free states in the plasma. This in turn affects the thermodynamic quantities known as the partition functions, which are required in the evaluation of the equilibrium concentrations of each of the species appearing in subroutine MAIN. A further discussion of this topic and a description of the modifications needed to account for these effects in subroutine MAIN is presented in the Appendix.

It must also be mentioned that screened Coulomb interactions cause a reduction in the plasma pressure from its ideal gas value. Hence an

alternative equation of state as given in reference [8] should be considered when calculating the chemical potential (μ , in equation (1)) of each species. Thus screened Coulomb interactions affect the chemical potentials of each species two-fold and Kovitya has ignored their effect in both cases. However, in a later section Kovitya has included the effect of screened Coulomb interactions when considering the collision cross-sections between charged particles, which are required for the evaluation of the transport coefficients of an ionised gas. This separate matter is discussed in section 8.

Kovitya has compared his results with the results of co-workers who have included the effect of screened Coulomb interactions using the Debye-Hückel approximation. Kovitya's conclusion is that the effect of the correction term on the partition functions is negligible. This is discussed later following a description of subroutine MAIN.

The approach used by the authors of the various railgun plasma-codes to evaluate the equilibrium concentration of each species is different from that used by Kovitya. Instead of using the variational principle, or the principle of the minimisation of the Gibb's free energy of the system, as subroutine MAIN does, they have used the Saha-Eggert system of equations to find the degree of ionisation of a railgun plasma. This approach, although different from the Gordon and McBride approach in that it assumes local thermal equilibrium within the plasma, also requires the evaluation of partition functions. Hence although the Debye-Hückel corrections mentioned previously should be applied to each of the species in a railgun plasma no authors have yet done so. In fact one of the weaknesses of Thio's Plasma Armature Rail Accelerator (PARA) code is that it considers only first ionisation although temperatures in excess of 30,000 K (where second ionisation becomes appreciable) are predicted. In order to overcome this limitation and since the plasma temperature is not known accurately anyway, Thio [9] has considered the plasma-armature temperature to be around 10,000 K. This, however, brings into question whether or not it is valid to assume, as Thio has done, that thermal conduction in the plasma-armature is negligible.

An added feature of the Gordon and McBride program is that it can determine the concentration of many different species although the user must stipulate the percentage contribution by weight or the number of moles of each species. This may be extremely useful for a railgun plasma where different species have been found to exist [6]. The applicability of the Gordon and McBride program is restricted by the range of validity of the ideal gas equation of state as pointed out by the authors [5]. This limitation, imposed by the ideal gas equation of state, is also likely to affect the validity of the railgun codes, which use the same assumption in the Saha-Eggert system of equations.

As mentioned earlier, the Gordon and McBride program (or rather subroutine MAIN in Kovitya's code) is based upon the minimisation of the Gibb's free energy. The Gibb's free energy for a system containing many different species j and with the number of particles allowed to vary is:

$$\Phi = \sum_j \mu_j N_j \quad (1)$$

where μ_j is the chemical potential of species j and N_j is the number of particles of species j . If the effect of a magnetic field is to be considered in equation (1) then this will mean that the chemical potential will include additional terms to account for the magnetic field. Whether these additional terms affect significantly the numerical results produced by subroutine MAIN is open to conjecture but care is required here because it may mean that the entire subroutine may have to be modified.

It must also be mentioned that the authors of the railgun plasma codes have not considered the effect of a magnetic field on the Saha equation predictions.

Much of the material presented in Kovitya's technical draft is an abridged version of the material in reference [5]. The reader is therefore advised to consult this reference for the details concerning the derivations of many of the non-standard thermodynamics equations which appear in Kovitya's technical draft. Unfortunately neither Kovitya nor Gordon and McBride explain the meaning of the expression 'mass-balance constraints.' This seems an alternative way of saying that the total number of ions and neutrals of a particular element is conserved regardless of the temperature and pressure of the ionised gas. This is a necessary condition if the assumption of chemical equilibrium is to hold.

4. DETERMINATION OF THE THERMOCHEMICAL FUNCTIONS

When the following thermodynamic functions are in the standard state, Kovitya refers to them as thermochemical functions. These are; using a modified terminology to that of Kovitya: (1) $C_p^{\circ}(T)$, the heat capacity at constant pressure, (2) the enthalpy $H(T)^{\circ}$ and (3) the entropy $S(T)^{\circ}$. The $^{\circ}$ superscript indicates that the standard state is being considered. According to Gordon and McBride, the standard state for a gas is the hypothetical ideal gas at unit fugacity, i.e. $\mu = 0$, whereas the standard state for a pure solid or liquid is the substance in the condensed phase at a pressure of one atmosphere.

Because the thermodynamic functions can be expressed in terms of the thermochemical functions for each of the species, i.e. $(C_p(T)^{\circ})_j$, $(H(T)^{\circ})_j$ and $(S(T)^{\circ})_j$, the problem of determining the thermodynamic functions becomes one of determining the thermochemical functions. The thermochemical functions are determined as functions of temperature using the method of least squares to fit a curve to several input values of these functions in the temperature range of 300 to 5000 K. The input values are obtained from the JANAF tables [10]. Thus polynomials with the following forms are obtained for each of the thermochemical functions:

$$\frac{C_p(T)^{\circ}}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4$$

$$\frac{H(T)^{\circ}}{RT} = a_1 + \frac{a_2 T}{2} + \frac{a_3 T^2}{3} + \frac{a_4 T^3}{4} + \frac{a_5 T^4}{5} + \frac{a_6}{T}$$

and

$$\frac{S(T)^{\circ}}{RT} = a_1 \ln T + a_2 T + \frac{a_2 T^2}{2} + \frac{a_4 T^3}{3} + \frac{a_5 T^4}{4} + a_7 \quad (2)$$

For each species two sets of coefficients are obtained in the two adjacent temperature intervals of 300 to 1000 K and 1000 to 5000 K. The polynomials are constrained to give equal values at 1000 K in order to eliminate any possible discontinuity at that point.

A separate program based upon an earlier but different program developed by Gordon and McBride [11] is used to evaluate the various coefficients appearing in equation (2). This program is called GENDAT.FOR and the data it produces, namely the coefficients of the thermochemical functions for each species, form the database which becomes part of the necessary input for the main program called JAN.FOR. It is JAN.FOR, which is used to evaluate the thermodynamic and transport properties of an ionised gas.

Neither Kovitya [1] nor Gordon and McBride [11] provide an explicit explanation as to why two temperature intervals are chosen for the evaluation of the thermochemical functions. In addition there is no explanation for choosing 1000 K to be the common temperature. Kovitya has suggested that these were chosen by the authors to ensure that at no stage would the calculated values deviate more than a few percent from the experimental values in the JANAF tables.

When Kovitya extended program GENDAT.FOR to higher temperatures (up to 30,000 K) he arbitrarily chose 15,000 K as the common temperature for the two adjacent temperature intervals.

The thermochemical functions for each species are determined by running program GENDAT.FOR separately with the appropriate input data for each species. The input data necessary to run the program consist of the values for the lowest and highest temperatures in the temperature range under consideration, the value for the common temperature, the enthalpy at absolute zero, the atomic mass and the total number of excitation levels for each species. In addition both the degeneracy factor and energy level for each excited state must be provided. These values are obtained from reference [11].

Kovitya presents the thermochemical functions for the various species that may comprise an ionised gas as functions of temperature beginning at equation (27) and ending at equation (54) in his technical draft. In this section of the draft all possible species are considered. These include ideal monatomic, ideal diatomic and ideal polyatomic species as well as corrections due to anharmonicity and vibration of the molecules. In this

form, however, the thermochemical functions are too complex to be handled by the main program JAN.FOR. That is JAN.FOR can only be used provided the equations for the thermochemical functions are specified in the form as given by equation (2). This is, as mentioned previously, the function of program GENDAT.FOR, which therefore re-casts Kovitya's equations (27) to (54) in the form given by equation (2).

5. RESULTS PRODUCED BY PROGRAM GENDAT.FOR

In this section the results of program GENDAT.FOR are presented for Cu and Cu^+ using different values for the common temperature between the adjacent temperature intervals. The number of excited energy levels used for the Cu case was 50 whereas for Cu^+ 55 levels were used. Many of the energy levels close to one another were lumped together with a larger degeneracy factor. This consideration of as many levels as possible represents a significant departure from the railgun plasma codes of Powell and Batteh [3] and Powell [4]. In these codes only 15 levels are considered because as the energy levels increase the partition functions decrease exponentially as a function of these levels. However the authors have ignored the fact that the degeneracy factors are increasing as well. As a result of this, program GENDAT.FOR has been written to consider up to as many as 60 energy levels.

Whether the approach adopted by Kovitya of lumping energy levels close to one another is correct or not is open to conjecture. An alternative (and probably more accurate) approach is given in Griem [7]. If this method was to be followed it would require modifications to be made to Kovitya's code.

The results for Cu^+ are presented in Table 1, while the results for Cu are presented in Table 2. Values chosen for the common temperature were 9000, 12000, 15000, 18000, 21000, 24000, 27000 and 30000 K. In each case two sets of coefficients were obtained, one corresponding to the lower temperature interval and the other to the higher temperature interval. As can be seen from the tables, each set of coefficients is markedly different even though they may be valid for an overlapping temperature interval. For instance, where the common temperature is chosen to be 4000 K the values of a_1 and a_2 for Cu^+ are 4.5110408 and $-3.4568627 \times 10^{-14} \text{ K}^{-1}$ respectively. Where the common temperature is 24000 K the values of a_1 and a_2 between 5000 and 24000 K are 9.5430612 and $-1.749684 \times 10^{-3} \text{ K}^{-1}$ respectively. The values of a_1 and a_2 are therefore vastly different even though both sets are valid over the overlapping temperature interval of 9000 to 24000 K. However, although this curve-fitting technique is unable to produce a unique set of coefficients for varying common temperatures, each set of coefficients produces good agreement with the input values for the thermochemical functions. These only deviated at most by a few percent from the input values.

6. THE MAIN PROGRAM JAN.FOR

Before discussing the main program JAN.FOR in detail, it is interesting to speculate whether the results of standard thermodynamics can be obtained when considering an ionised gas to be composed only of an ideal monatomic species. In standard thermodynamics the heat capacity at constant pressure for such an ideal gas is $5/2 nR$ where n is the number of moles and R is the universal gas constant. Hence the ratio (γ) of the heat capacity at constant pressure to that at constant volume becomes $5/3$. Although Kovitya has used the ideal gas equation of state in the main program the value of $5/3$ for γ will not be obtained. There are two major reasons for this.

The first reason is that when considering an ionised gas to be composed of an ideal monatomic species Kovitya includes an additional component to account for the electrons in the total heat capacity for the ionised gas. This extra contribution which appears as equation (29) in Kovitya's technical draft is:

$$\frac{C_p(T)_{el}}{R} = \frac{\sum_i g_i \left(\frac{\epsilon_i}{kT}\right)^2 e^{-\epsilon_i/kT}}{\sum_i g_i e^{-\epsilon_i/kT}} - \left[\frac{\sum_i g_i \frac{\epsilon_i}{kT} e^{-\epsilon_i/kT}}{\sum_i g_i e^{-\epsilon_i/kT}} \right]^2 \quad (3)$$

where g_i and ϵ_i are the degeneracy factor and energy for the i -th excited level and k is the Boltzmann constant. The 'el' subscript denotes that equation (3) is the electron contribution to the total heat capacity. According to the literature, equation (3) should take effect for temperatures in excess of 10,000 K.

The second reason is that the actual heat capacity of most interest is the heat capacity of the entire mixture. This now consists of two heat capacities, one representing the physical quantity described in the previous paragraph and the other known as the reaction heat capacity. The total heat capacity at constant pressure for a plasma mixture is represented by the following equation, which appears as equation (11) in Kovitya's technical draft:

$$C_p(T) = \sum_{j=1}^N n_j (C_p(T))^0_j + \sum_{j=1}^N n_j (H(T))^0_j \left(\frac{\partial \ln n_j}{\partial \ln T} \right)_p / T \quad (4)$$

In the above equation the reaction heat-capacity is given by the second expression on the right hand side. This term will not contribute if the number of moles of each species n_j are independent of the temperature T .

Whilst Kovitya has not provided a sensitivity analysis concerning program GENDAT.FOR he does provide an indication of the effect of the Debye-Hückel corrections in a hydrogen plasma, which arise as a result of plasma polarisation [7]. In that section of his technical draft Kovitya has used the main program to evaluate the chemical equilibrium composition of the various species, e.g. H-atoms, H^+ -ions and electrons at a pressure of one atmosphere. Then comparisons are made with the results of Patch [12], who has considered the effect of the Debye-Hückel approximation. The only area of disagreement between Patch and Kovitya occurs in the evaluation of the number of H-atoms for temperatures above 20,000 K. However at these temperatures the plasma is so strongly ionised that the number of (neutral) H-atoms is very small (about a factor of 10^3 less) in comparison to the number of H^+ -ions or to the number of electrons. Hence even though there is disagreement between the two methods for higher temperatures it represents a negligible effect anyway. This leads Kovitya to conclude that the Debye-Hückel approximation has very little effect on his results.

However it is considered that this conclusion is not valid for higher pressures. According to Patch [12], for pressures approaching 1000 atmospheres the ideal gas approximation used by Kovitya is inadequate for crude (± 40 percent) calculations of compositions. This has been supported by Kovitya in separate discussions. Therefore subroutine MAIN in program JAN.FOR should be modified to take into account plasma polarisation effects for higher pressures.

7. TRANSPORT PROPERTIES

Program JAN.FOR is actually a modified version of the TRAN 72 NASA code written by Svehla and McBride [13]. This program in its original form was restricted to the evaluation of the transport properties of a weakly-ionised gas and did not evaluate the electrical conductivity. Because Kovitya was interested in evaluating the transport properties for strongly-ionised plasmas (as well as weakly-ionised ones) he had to modify the TRAN 72 code. These modifications involve the consideration of higher order approximations of the Chapman-Enskog theory so that more accurate values for the kinematic coefficient of viscosity and for the electrical and thermal conductivities can be obtained.

7.1 Viscosity

Although this parameter is not likely to be required for railgun work it is dealt with briefly for the sake of completeness. In order to determine the overall viscosity η of an ionised gas, Kovitya uses a method of averaging where the viscosities of each species are added together according to that species' mole-fraction within the gas. The viscosity for each species is determined from equations (59) + (61) of Kovitya's technical draft. These equations are very complex and show that the viscosity is dependent on the averaged collision cross-sections, which are defined as follows:

$$\bar{\Omega}_{ij}^{(l,s)} = \frac{\bar{Q}_{ij}^{(l,s)}}{\pi} = \frac{2(l+1)}{\pi(s+1)!(2l+1-(-1)^l)} \int_0^\infty e^{-E/kT} \left(\frac{E}{kT}\right)^{s+1} Q^{(l)}(E) d\left(\frac{E}{kT}\right) \quad (4)$$

where

$$Q^{(l)}(E) = 2\pi \int_0^\infty (1 - \cos^l \theta) b \, db \quad (5)$$

In the above, E is the relative energy of the colliding particles, θ is the deflection angle and b is the impact parameter.

The deflection angle is itself a function of the relative energy and impact parameter. It is given by:

$$\theta(b, E) = \pi - 2b \int_{r_0}^\infty \left(1 - \frac{b^2}{r^2} - \frac{V(r)}{E}\right)^{-1/2} \frac{dr}{r^2} \quad (6)$$

where $V(r)$ is the interaction potential and r_0 is the outermost root of

$$1 - \frac{b^2}{r_0^2} - \frac{V(r_0)}{E} = 0 \quad (7)$$

7.2 Thermal Conductivity

The thermal conductivity λ is defined as the sum of three components known as the internal, reaction and translation thermal conductivities. The expressions for each of these thermal conductivities given in Kovitya's technical draft has been taken from reference [13]. According to Svehla and McBride, the reaction thermal conductivity $\lambda_{\text{reaction}}$ only contributes if chemical reactions are occurring within the plasma mixture. The internal thermal conductivity λ_{int} represents the internal energy contribution of a species to the thermal conductivity. When a plasma mixture consists of inert monatomic species without internal structure then the total thermal conductivity is given solely by the translation thermal conductivity $\lambda_{\text{monatomic}}$.

Expressions for the thermal conductivities appear in equations (62) to (78) of Kovitya's technical draft. However there is no guide as to the assumptions used in deriving these equations and also no indication of their range of validity.

The reaction-dependent thermal conductivity component is presented in equations (64) to (68). This conductivity can only be found if the stoichiometric coefficients for each of the chemical reactions have been determined. The stoichiometric coefficients are evaluated in subroutine INPUT of the main program.

As mentioned earlier Kovitya had to extend the TRAN 72 code to take strong ionisation into account. The first instance of this extension appears in the evaluation of the translation thermal conductivity, which is now the sum of two independent contributions; one due to heavy particle collisions described by equations (70) - (74) and the other due to electron collisions. In order to evaluate the contribution due to electron collisions higher order approximations of the Chapman-Enskog theory are required but Kovitya stops at the third order approximation as demonstrated by equation (75). In the regions where even higher order approximations must be considered for the electron contribution, Kovitya suggests that the heavy particle collision contribution may dominate the electron collision contribution thereby disposing of the need to consider higher orders. When the electron collision term is important, i.e. at high temperatures, then the third order approximation for the electron collision translation thermal conductivity referred to as λ_e by Kovitya shows less than a one percent deviation from the fourth order approximation. Kovitya therefore concluded that the third order approximation is sufficient.

7.3 Electrical Conductivity

Kovitya stops at the second order approximation of the Chapman-Enskog theory in the evaluation of the electrical conductivity which is given by:

$$[\sigma_2] = \frac{3x_e e^2}{16 kT} \left(\frac{2\pi RT}{m_e} \right)^{1/2} \left(\frac{1}{q^{00} - (q^{01})^2 / q^{11}} \right) \quad (8)$$

In equation (8), m_e represents the electron mass and x_e is the electron mole fraction. In addition, the following terms are used:-

$$\begin{aligned} q^{00} &= \sum_{\substack{j=1 \\ j \neq e}}^n x_j \bar{Q}_{ej}^{(1,1)}, \\ q^{01} &= \sum_{\substack{j=1 \\ j \neq e}}^n x_j \left(\frac{5}{2} \bar{Q}_{ej}^{(1,1)} - 3 \bar{Q}_{ej}^{(1,2)} \right) \\ \text{and } q^{11} &= \sqrt{2} x_e \bar{Q}_{ee}^{(2,2)} + \sum_{\substack{j \neq e \\ j=1}}^n x_j \left(\frac{25}{4} \bar{Q}_{ej}^{(1,1)} - \frac{315}{8} \bar{Q}_{ej}^{(1,2)} + 57 \bar{Q}_{ej}^{(1,3)} - 30 \bar{Q}_{ej}^{(1,4)} \right) \end{aligned} \quad (9)$$

In the above equations, x_j is the mole fraction of species j .

Kovitya's justification for stopping at the second order is that the electrical conductivity exhibits a maximum deviation of 0.2% from the fourth order approximation in the temperature range of 3,500 to 20,000 K. When the plasma mixture is strongly ionised, as occurs for temperatures above 20,000 K and for pressures around one atmosphere, the electrical conductivity is given by the Spitzer-Harm expression [14].

8. COLLISION CROSS-SECTIONS

Each of the transport coefficients has a dependence on the collision cross-sections between the various species. The integral form for the collision cross-sections has already been given by equation (4). In general these integrals are intractable mainly because the deflection angle for collisions is itself defined by an integral as demonstrated by equation (6). This integral can only be solved with a proper knowledge of the interaction potential $V(r)$ between colliding particles. Even when the interaction potential is known, e.g. for charged particles in a plasma the shielded Coulomb potential is used and for molecules the Lennard-Jones potential is appropriate, the cross-section integrals can only be solved numerically.

Four distinct types of collision exist. These are: (1) collisions between neutral particles or neutral-neutral collisions, (2) neutral-ion collisions, (3) electron-neutral collisions and (4) collisions between charged particles. Kovitya suggests that cross-sections involving neutral particles cannot be neglected for high temperature plasma mixtures if the pressure is very high as it is in a railgun.

For each type of collision a different interaction potential must be used. In the case of neutral-neutral encounters the Lennard-Jones potential is used in the calculations of neutral-neutral cross-sections. This potential is given by:

$$V(r) = 4\epsilon \left[\left(\frac{\sigma_s}{r} \right)^{12} - \left(\frac{\sigma_s}{r} \right)^6 \right] \quad (10)$$

where r is the distance between particles and σ_s and ϵ represent the force constants of the potential. Values of the force constants are supplied in subroutine TRANSP, which is the subroutine of program JAN.FOR largely responsible for the evaluation of the transport coefficients. These values may not be very accurate in some cases because estimates have only been provided in the absence of hard data.

Neutral-ion collision cross-sections are dominated by charge exchange at high energies while at low energies they are dominated by an r^{-4} polarisation potential. Many of the values used in determining these cross-sections have been found experimentally.

Except for a few special cases where the experimental data are known, the momentum transfer cross-sections for electron-neutral interactions are estimated by assuming that the cross-sections are independent of energy. According to Kovitya this assumption is probably highly inaccurate but must be accepted at this stage because of the scarcity of experimental data. The simple approximation methods employed here mean that the values of the electrical conductivity for a weakly-ionised gas are not likely to be accurate. The problem is not so serious for high temperatures because electron-ion interactions begin to dominate over electron-neutral interactions. A better approximation for evaluating the cross-sections for electron-neutral interactions is the Born approximation which requires a knowledge of the interaction potential between electrons and neutral particles.

For interactions between charged particles, the screened Coulomb potential is used as the interaction potential. As mentioned previously cross-sections involving the screened Coulomb potential have been calculated assuming that the 'cut-off' distance for binary collisions is equal to the Debye length. The various collision integrals are calculated within program JAN.FOR by the use of sixth-order polynomials, which are found using the method of least squares fitted to published data.

When calculating the electrical conductivity Kovitya adjusts the collision cross-section integral for electron-electron collisions in the second order Chapman-Enskog approximation to give the Spitzer-Harm result for electrical conductivity at full ionisation [14]. This means the electron-electron collision cross-section becomes:

$$Q_{ee}^{(2,2)} = \left(\frac{1}{\gamma_{sp}} - 1 \right) \sum_{j=1}^m x_j^{(+)} Q_{ej}^{(2,2)} / \sum_{j=1}^m x_j^{(+)} \quad (11)$$

where $x_j^{(+)}$ is the mole fraction of the j -th positive ionic species and γ_{sp} is a function of the average charge number squared, \bar{Z} , which in turn is given by:

$$\bar{Z} = \sum_{j=1}^m x_j^{(+)} Z_j^2 / x_e \quad (12)$$

where Z_j is the ionic charge number. By fitting a curve to experimental data in reference [14] Kovitya finds that:

$$\gamma_{sp} = 0.14523 \ln \bar{Z} + 0.582, \quad 1 < \bar{Z} < 4 \quad (13)$$

If the effect of a magnetic field is to be considered in the evaluation of the electrical conductivity then extra terms begin to appear in the expression for the electrical conductivity. Whether these are significant or not is open to conjecture. In fact the inclusion of the effect of a magnetic field may require a re-formulation of the Chapman-Enskog theory in addition to modifying the collision cross-section integrals. Such detail is beyond the scope of this report.

9. INPUT TO PROGRAM JAN.FOR

Input to the main program is supplied from two data files, one called FORØ15.DAT and the other called THERMO.DAT. The data in FORØ15.DAT must be typed in the manner as prescribed in reference [13]. Reference [13] also contains examples using different input data. THERMO.DAT is the database containing the coefficients of the thermochemical functions for various species, which are evaluated by program GENDAT.FOR.

10. MODIFICATIONS TO THE TRAN 72 CODE

The flow chart for the TRAN 72 code is shown in figure 1. In this figure the dashed circles represent sections of the code, which do not appear in programs JAN.FOR. This means that subroutines ROCKET, RKOUT, FROZEN, SHCK and DETON from the original TRAN 72 code are not required in the evaluation of thermodynamic and transport properties of ionised gases.

In general most of the subroutines appearing in JAN.FOR have been altered only slightly from their original form in the TRAN 72 code and thus their functions remain essentially the same as described in reference [13]. The only significant changes to the subroutines occur in subroutines INPUT, which prepares the input for the calculation of the transport coefficients and TRANSP, which calculates the transport coefficients. TRANSP has been altered so that the electrical conductivity can now be evaluated while INPUT has been altered to include charge-charge interactions. For the later alteration to be effected, Kovitya has created two new subroutines called CS1 and CS2.

11. SAMPLE RESULTS

In this section the results of the main program JAN.FOR produced by the VAX 11/780 computer at MRL are discussed and mention is also made of the comparison of the VAX results with those provided by Kovitya, who has generated his results using the CSIRO Cyber 7600 computer. The results generated by the VAX 11/780 appear in tables 3,4 and 5 and are in excellent agreement with those obtained by Kovitya.

The input data used to produce the results for the necessary comparison were identical for both machines. The comparison was made for an ionised gas composed entirely of copper and the coefficients chosen for the thermochemical functions were those obtained by running GENDAT.FOR on the Cyber 7600. The coefficients of each species appeared in a data file named THERMO.DAT. Pressures ranged between one and 1000 atmospheres whilst temperatures ranged between 5000 and 26000 K. A summary of the results generated by the VAX 11/780 appears in the tables.

As mentioned previously, the agreement between both sets of results was excellent. In most cases there was no difference between the results for the physical quantities listed in the tables generated by both computers. If a difference did exist it invariably occurred in the fourth significant figure of a thermodynamic or transport property.

A major draw-back to this code becoming an alternative to the railgun plasma codes is that the user must specify an equilibrium pressure as well as an equilibrium temperature. These are properties which are calculated in the railgun plasma codes from the equations of magnetohydrodynamics and from the equation of state. In point of fact, Batteh and Powell [2,3] allow the temperature and pressure to vary quite markedly over the plasma dimensions they are considering. However, if Kovitya's work is to be applied to a railgun plasma the user must know in advance the average temperature and average pressure of a railgun plasma. This therefore requires either the use of the railgun codes to find the average temperatures and average pressures or a separate code, which calculates these properties.

A surprising feature of table 4 is that the mole fraction of neutral copper is quite high for the high temperature and high pressure plasma. This indicates that a plasma under these conditions is not completely ionised as previously thought. This result casts doubt on the validity of using the Spitzer formula to evaluate the electrical conductivity of a railgun plasma. Thus Kovitya's decision to consider interactions involving neutral particles when evaluating the collision cross-sections which are needed to evaluate the electrical conductivity seems vindicated. Consideration will be given in the future to incorporating the equations used by Kovitya to evaluate the electrical conductivity into the railgun plasma codes written by Powell and Batteh [2,3] and also by Thio.

12. CONCLUSION

This report has examined the work of Kovitya, who has developed two computer codes for predicting many of the physical properties of an ionised gas. The first of these codes is called GENDAT.FOR and is used to find polynomial expressions for the thermochemical functions of enthalpy, entropy and specific heat. The second code is called JAN.FOR. This code uses the results generated by GENDAT.FOR to predict the thermodynamic and transport properties of an ionised gas.

Attention has centred on the validity of Kovitya's assumptions and models for predicting the properties of a railgun plasma and has involved making comparisons with the assumptions and models used by the authors of current railgun plasma codes.

It has been shown that the coefficients for the polynomial expressions obtained from GENDAT.FOR vary quite substantially when a different common temperature was chosen in the temperature range of interest. However this variation does not appear to be serious since at no stage did the values

for the thermochemical functions (computed from the various coefficient sets) vary more than a few percent from the input values obtained from the JANAF tables [10]. Since there is no dependence on each of the coefficients individually in program JAN.FOR it is expected that the different sets of coefficients when used in JAN.FOR will not affect the predictions of the thermodynamic and transport properties of an ionised gas.

If JAN.FOR is to be extended to include temperatures up to 60,000K, which is the maximum likely temperature to be met in EML work then modifications to the code are required. When considering temperatures above 20,000K and/or pressures much greater than one atmosphere, it becomes necessary to include the effect of screened Coulomb interactions. In addition another equation of state as given in reference [8] should be considered instead of the ideal gas equation of state. These modifications would have to be introduced into subroutine MAIN of program JAN.FOR and would affect the chemical potential of each species in the ionised gas. This in turn would affect the results for the thermodynamic and transport properties since the composition of the ionised gas would now be altered.

Once modifications to include higher temperatures and pressures have been made it would be necessary to compare the results for the electrical conductivity predicted by JAN.FOR with those of the various available railgun plasma codes [2,3,4] for the same plasma conditions. The electrical conductivities may be substantially different as Kovitya's code predicts a fairly high concentration of neutral particles at high temperatures and pressures. The effect of neutral particles on the electrical conductivity has been neglected by the authors of the railgun plasma codes. If interactions with neutral particles cause significant differences between the values for the electrical conductivities predicted by Kovitya's code and the railgun plasma codes it may then be necessary to incorporate techniques used by Kovitya into the railgun codes. However, this requires further investigation because even though Kovitya has included the effect of interactions with neutral particles, his evaluation of the collision cross-sections for cases where there is no experimental data is necessarily based on crude approximations. Thus for an ionised gas containing a substantial number of neutral particles the values for the electrical conductivity predicted by JAN.FOR are not likely to be accurate. Further improvement to Kovitya's code is also required here.

It is therefore considered that in its present form JAN.FOR is of limited use in predicting the physical properties of a railgun plasma and does not offer substantially better results than the existing railgun codes. A difficulty arising in the use of JAN.FOR is that the user must specify the temperature and pressure of the plasma input data whereas these are calculated by the railgun codes. Although modifications would be required to make JAN.FOR more applicable to railgun plasmas some of the techniques used by Kovitya could perhaps be incorporated as further improvements to the railgun codes.

13. ACKNOWLEDGEMENTS

The author wishes to express his deep gratitude to Dr P. Kovitya of the CSIRO Division of Applied Physics for making his draft report available for examination and for his patient willingness to discuss all aspects of the work.

The author also wishes to acknowledge the initiative of Dr R.A. Marshall, who first proposed that the applicability of Dr Kovitya's work to railgun plasmas should be examined.

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T A B L E 1

Results for Cu^+

Temp. Interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
5000-9000	1.3115619×10^1	$-2.5113464 \times 10^{-3}$	6.8479610×10^{-8}	$2.3171861 \times 10^{-11}$	$-1.5458911 \times 10^{-15}$	-4.2344191×10^3	-6.753494×10^1
9000-30000	4.5110408	$-3.4568627 \times 10^{-4}$	2.2869173×10^{-8}	$-6.7286654 \times 10^{-12}$	$7.36611652 \times 10^{-18}$	1.7348597×10^4	-3.5876028
5000-12000	1.4368496×10^1	$-3.7586112 \times 10^{-3}$	4.512233×10^{-7}	$2.3574355 \times 10^{-16}$	$4.4061442 \times 10^{-11}$	-1.8069381×10^3	-7.511882×10^1
12000-30000	3.4855376	$-1.3324569 \times 10^{-4}$	7.00829×10^{-9}	$-1.6431614 \times 10^{-13}$	$1.4259056 \times 10^{-18}$	2.4129285×10^4	4.3727981
5000-15000	1.3875214×10^1	$-3.5919425 \times 10^{-3}$	4.3714026×10^{-7}	$2.3795303 \times 10^{-11}$	$4.8466302 \times 10^{-16}$	2.1700492×10^3	-7.1573333×10^1
15000-30000	2.957165	$-4.3211262 \times 10^{-5}$	1.1987093×10^{-9}	$-1.4683019 \times 10^{-15}$	$-2.5182907 \times 10^{-19}$	2.9370215×10^4	8.4157099
5000-18000	1.221196×10^1	-2.837697×10^{-3}	3.1588172×10^{-7}	$1.5557436 \times 10^{-11}$	2.838988×10^{-16}	7.9447238×10^3	-5.9976675×10^1
18000-30000	2.7975093×10^1	$-1.9224303 \times 10^{-5}$	$9.5341544 \times 10^{-11}$	$1.7696391 \times 10^{-14}$	$-3.3236481 \times 10^{-19}$	3.3361963×10^4	9.8734925
5000-21000	1.0719581×10^1	$-2.2095331 \times 10^{-3}$	2.2361101×10^{-7}	$9.9095308 \times 10^{-12}$	$1.6132853 \times 10^{-16}$	1.3584449×10^4	-4.9472563×10^1
21000-30000	2.7292474	$-1.2870071 \times 10^{-5}$	$-1.0172946 \times 10^{-11}$	$1.3310438 \times 10^{-14}$	$-2.197973 \times 10^{-19}$	3.6840779×10^4	1.0450717×10^1
5000-24000	9.5430612	$-1.7496843 \times 10^{-3}$	1.6185795×10^{-7}	$6.4975903 \times 10^{-12}$	9.514695×10^{-17}	1.8789611×10^4	-4.1114458×10^1
24000-30000	2.7028607	-1.084631×10^{-5}	$1.3073638 \times 10^{-11}$	$1.0591925 \times 10^{-14}$	$-1.6830811 \times 10^{-19}$	4.0047986×10^4	1.0677366×10^1
5000-27000	8.6253836	$-1.4145786 \times 10^{-3}$	1.2042600×10^{-7}	$4.4137874 \times 10^{-12}$	$5.8658977 \times 10^{-17}$	2.3602276×10^4	-3.4540365×10^1
27000-30000	2.37879614	1.2165445×10^{-5}	$-9.4466178 \times 10^{-11}$	$-1.4208257 \times 10^{-14}$	$2.8529728 \times 10^{-19}$	4.5689732×10^4	1.3401269×10^1
5000-30000	7.9003464	$-1.1657955 \times 10^{-3}$	9.1916102×10^{-8}	$3.0981616 \times 10^{-12}$	3.767254×10^{-17}	2.8104019×10^4	-2.9306912×10^1
30000	2.5153684	$1.6406993 \times 10^{-11}$	$-1.3077243 \times 10^{-16}$	$-1.7150556 \times 10^{-20}$	$4.5785362 \times 10^{-25}$	4.8001136×10^4	1.2340187×10^1

T A B L E 2

Results for Cu

Temp. Interval (K)	a_1	a_2	a_3	a_4	a_5	a_6	a_7
5000-9000	2.2604407	6.1362944×10^{-4}	$-6.3922916 \times 10^{-8}$	6.911143×10^{-14}	$3.3508936 \times 10^{-16}$	7.3870784×10^3	6.1068027
9000-30000	1.1930785×10^1	3.6101229×10^{-3}	$-2.5179216 \times 10^{-6}$	$7.0684591 \times 10^{-12}$	$-7.0692059 \times 10^{-17}$	5.2713865×10^4	1.1492263×10^2
5000-12000	2.1061085	1.1697553×10^{-3}	$-2.8858297 \times 10^{-7}$	$3.1241292 \times 10^{-11}$	$-1.0933329 \times 10^{-15}$	9.5979812×10^3	6.3750262
12000-30000	1.0456612×10^1	3.3107208×10^{-3}	$-2.2967928 \times 10^{-7}$	$6.3656808 \times 10^{-12}$	$-6.2562347 \times 10^{-17}$	4.9930009×10^4	1.034246×10^2
5000-15000	6.85267	$-1.2882645 \times 10^{-3}$	1.7049789×10^{-7}	$5.4720641 \times 10^{-12}$	$-2.9873997 \times 10^{-17}$	5.5263164×10^3	-2.613545×10^1
15000-30000	5.9200577	4.3277951×10^{-4}	$-4.4856605 \times 10^{-8}$	$1.2093773 \times 10^{-12}$	$-9.6937965 \times 10^{-18}$	-1.9456137×10^4	-2.6528052×10^1
5000-18000	1.0207484×10^1	$-2.8914460 \times 10^{-3}$	3.1588172×10^{-7}	$1.5557436 \times 10^{-11}$	2.838988×10^{-16}	7.9447238×10^3	-5.9976675×10^1
18000-30000	1.2387997	$-4.4256021 \times 10^{-4}$	$-4.2217627 \times 10^{-9}$	$4.8974542 \times 10^{-13}$	$-6.4467888 \times 10^{-18}$	5.2310565×10^4	-7.9408766×10^1
5000-21000	9.2351146	$-2.4969474 \times 10^{-3}$	3.8688793×10^{-7}	$2.1669617 \times 10^{-11}$	$3.9993705 \times 10^{-16}$	8.0005720×10^3	-4.2479837×10^1
21000-30000	1.353129×10^1	$-5.5445843 \times 10^{-4}$	1.8426233×10^{-9}	$5.4052327 \times 10^{-13}$	$-8.0533213 \times 10^{-18}$	5.7134482×10^4	-8.9039852×10^1
5000-24000	6.2130081	$-1.3129128 \times 10^{-3}$	2.2752578×10^{-7}	$1.2842375 \times 10^{-11}$	$2.2828143 \times 10^{-16}$	1.6671634×10^4	-2.1018416×10^1
24000-30000	1.4006558×10^1	$-5.9554363 \times 10^{-4}$	$-1.2174069 \times 10^{-9}$	$5.6621948 \times 10^{-13}$	$-8.6698254 \times 10^{-18}$	5.7738958×10^4	-9.3094612×10^1
5000-27000	3.1028056	$-1.7184216 \times 10^{-4}$	8.5788602×10^{-8}	$5.6815942 \times 10^{-12}$	$1.0237187 \times 10^{-16}$	2.5797682×10^4	1.2480755
27000-30000	4.9399762	7.8818226×10^{-4}	$-6.1422294 \times 10^{-9}$	$-9.2099382 \times 10^{-13}$	$1.8518722 \times 10^{-17}$	1.0432906×10^5	7.0807986×10^1
5000-30000	7.027566×10^{-1}	6.5565525×10^{-4}	$-9.4887678 \times 10^{-9}$	$1.2668937 \times 10^{-12}$	3.170883×10^{-17}	3.3743345×10^4	1.8561154×10^1
30000	2.3105452	$-4.4398962 \times 10^{-11}$	$1.9028417 \times 10^{-16}$	4864617×10^{-20}	$-1.2023002 \times 10^{-24}$	6.2714585×10^4	2.0962924

T A B L E 3

Thermodynamic Properties - Results produced by the VAX 11/780

P (atm)	1.0000	1.0000	10.000	100.00	1000.00	10000.00	100000.00	1000000.00
T (K)	5000	8000	11000	14000	17000	20000	23000	26000
ρ (g/cm ³)	1.5448 x 10 ⁻⁴	8.4311 x 10 ⁻⁵	5.3677 x 10 ⁻⁵	4.2012 x 10 ⁻³	2.8654 x 10 ⁻³	2.8093 x 10 ⁻²	2.1788 x 10 ⁻²	1.7473 x 10 ⁻²
h (cal/g)	1723.6	2611.5	3729.4	4345.1	6011.8	5748.3	7082.0	8556.0
s (cal/(g)(K))	0.8680	0.9994	1.0296	0.9844	1.0923	0.9712	1.0332	1.0934
M	63.380	55.345	48.450	48.263	39.971	46.104	41.121	37.278
$(\partial \ln v / \partial \ln p)_T$	-1.00211	-1.06312	-1.10731	-1.10843	-1.12170	-1.11836	-1.12723	-1.11753
$(\partial \ln v / \partial \ln T)_p$	1.0341	1.8620	2.1499	1.9449	1.9079	1.7962	1.8228	1.7698
C_p (cal/(g)(K))	0.1444	0.5808	0.7004	0.5389	0.5445	0.4196	0.4690	0.5127
$\gamma = C_p / C_v$	1.2989	1.1782	1.1953	1.2204	1.2669	1.2708	1.2741	1.2628
a (m/s)	923.0	1189.9	1502.1	1715.6	2116.6	2140.9	2434.2	2706.1

TABLE 4

Mole Fractions - Results produced by VAX 11/780

P (atm)	1.0000	1.0000	10.000	100.00	100.00	100.00	1000.00	1000.00
T (K)	5000	8000	11000	14000	17000	20000	23000	
Cu	9.9326×10^{-1}	7.4198×10^{-1}	5.2492×10^{-1}	5.1888×10^{-1}	2.5865×10^{-1}	4.5139×10^{-1}	2.9694×10^{-1}	
Cu+	3.0858×10^{-3}	1.2899×10^{-1}	2.3752×10^{-1}	2.4048×10^{-1}	3.6985×10^{-1}	2.7349×10^{-1}	3.4750×10^{-1}	
Cu++	2.826×10^{-17}	3.797×10^{-9}	1.831×10^{-6}	2.323×10^{-5}	5.460×10^{-4}	5.104×10^{-4}	2.675×10^{-3}	
Cu+++	0.0	1.313×10^{-27}	1.710×10^{-19}	1.694×10^{-15}	9.499×10^{-12}	7.964×10^{-11}	7.474×10^{-9}	
Cu2	5.647×10^{-4}	2.743×10^{-5}	3.072×10^{-5}	9.127×10^{-5}	8.168×10^{-6}	1.048×10^{-4}	2.203×10^{-5}	
E	3.0858×10^{-3}	1.2899×10^{-1}	2.3753×10^{-1}	2.4053×10^{-1}	3.7094×10^{-1}	2.7451×10^{-1}	3.5285×10^{-1}	

T A B L E 5

Transport Properties - Results produced by the VAX 11/780

P (atm)	1.0000	1.0000	10.000	100.00	100.00	1000.00
T (K)	5000	8000	11000	14000	17000	20000
η (poise)	2268.0 x 10 ⁻⁶	1544.0 x 10 ⁻⁶	1241.0 x 10 ⁻⁶	1958.0 x 10 ⁻⁶	1240.0 x 10 ⁻⁶	3157.0 x 10 ⁻⁶
$\lambda_{\text{monatomic}}$ (J/cm-sec K)	1374.0 x 10 ⁻⁶	3797.0 x 10 ⁻⁶	9947.0 x 10 ⁻⁶	21395.0 x 10 ⁻⁶	35932.0 x 10 ⁻⁶	55204.0 x 10 ⁻⁶
λ_{int} (J/cm-sec K)	562.0 x 10 ⁻⁶	374.0 x 10 ⁻⁶	353.0 x 10 ⁻⁶	465.0 x 10 ⁻⁶	261.0 x 10 ⁻⁶	387.0 x 10 ⁻⁶
λ_{frozen} (J/cm-sec K)	1935.0 x 10 ⁻⁶	4171.0 x 10 ⁻⁶	10300.0 x 10 ⁻⁶	21860.0 x 10 ⁻⁶	36192.0 x 10 ⁻⁶	55591.0 x 10 ⁻⁶
$\lambda_{\text{reaction}}$ (J/cm-sec K)	48.0 x 10 ⁻⁶	1056.0 x 10 ⁻⁶	1349.0 x 10 ⁻⁶	1049.0 x 10 ⁻⁶	979.0 x 10 ⁻⁶	886.0 x 10 ⁻⁶
λ (J/cm-sec K)	1984.0 x 10 ⁻⁶	5227.0 x 10 ⁻⁶	11649.0 x 10 ⁻⁶	22909.0 x 10 ⁻⁶	37171.0 x 10 ⁻⁶	56477.0 x 10 ⁻⁶
$C_{p,\text{frozen}}$ (J/g K)	0.5210	0.6611	0.8157	0.8357	0.8632	0.7863
$C_{p,\text{eq}}$ (J/g K)	0.6042	2.4299	2.9305	2.2546	2.2782	1.7554
$[\sigma]_2$ (s/cm)	4.0835	30.83	65.86	108.0	155.2	190.7

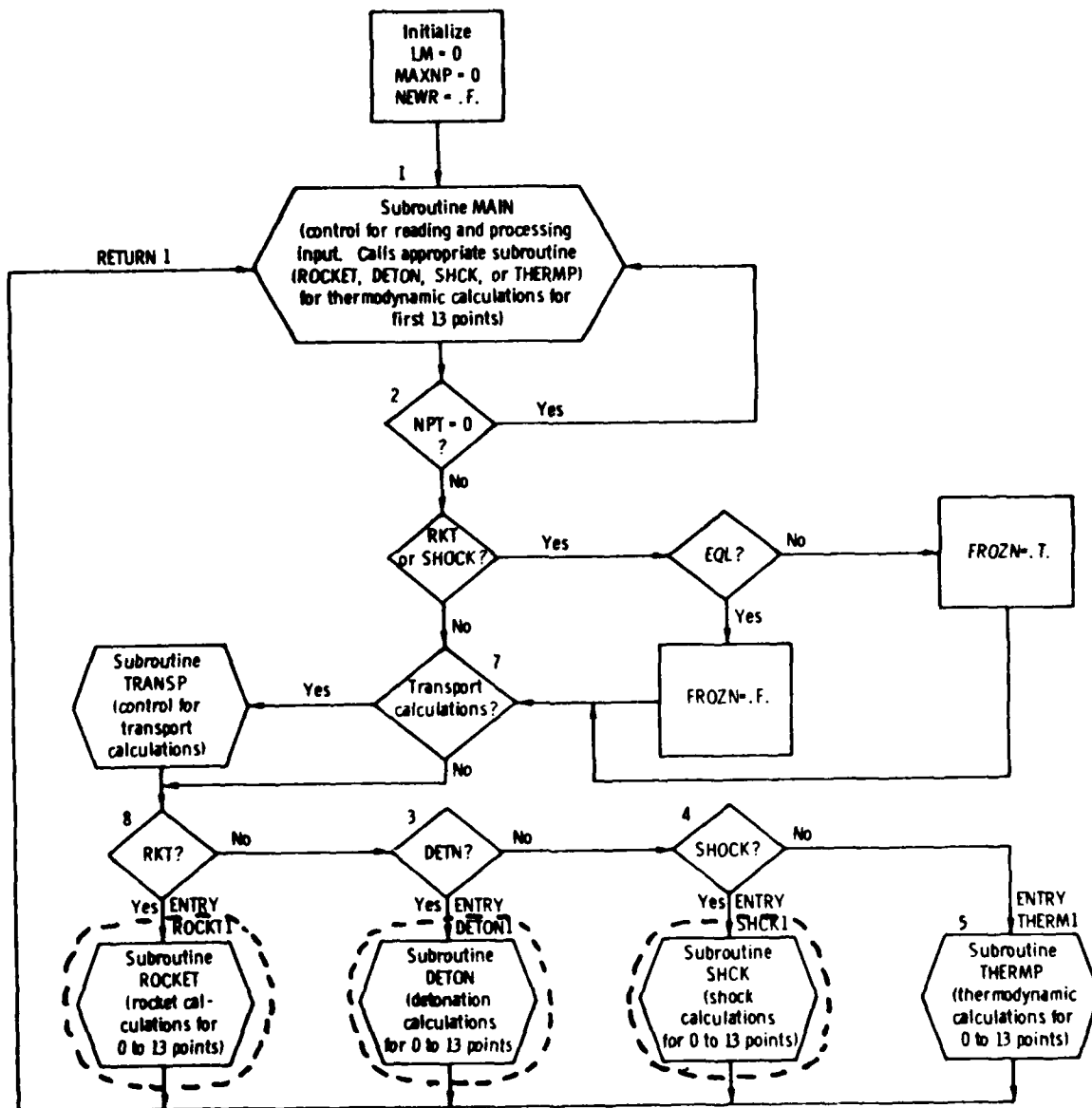


FIGURE 1 Flowchart for the TRAN 72 code.

APPENDIX

SCREENED COULOMB INTERACTIONS

As mentioned in section 3, screened Coulomb interactions affect the partition functions of each species of an ionised gas as well as the plasma pressure. In this appendix a description of the modifications which would need to be made to account for these interactions in subroutine MAIN is presented.

According to Greim [7], instead of considering the effect of screened Coulomb interactions on the partition functions and hence the compositions of each species in an ionised gas, one can consider the reduction of the ionisation energy in a purely thermodynamic manner. By thermodynamic manner it is meant that the free energy (equation (1)) must assume an extremum because the auxiliary conditions for equilibrium are that the temperature and mass (and hence the specific volume) are fixed. Thus corrections can be made to the chemical potentials of each species rather than their chemical compositions provided the Gibbs free energy assumes an extremum. This is precisely the case in subroutine MAIN where the Gibbs free energy is minimised. Therefore the effect of screened Coulomb interactions can be applied to the chemical potentials of each of the species rather than their chemical compositions.

As indicated also by Griem, there are many approximations and models which can account for screened Coulomb interactions. These include the ion-sphere model, the nearest-neighbour approximation and the Debye-Hückel approximation. The last of these approximations is the most commonly used.

In the absence of screened Coulomb interactions, the chemical potential of each species j is defined as:

$$\mu_j = \mu_j^{\circ} + RT \ln (n_j/n) + RT \ln (P/101.3) \quad (\text{A-1})$$

where R is the universal gas constant, T is the temperature and P is the pressure in kPa. Here μ_j° is the chemical potential of each species in the standard state, which is defined by the following equation:

$$\mu_j^{\circ} = H(T)_j^{\circ} - T S(T)_j^{\circ} \quad (\text{A-2})$$

In writing down equation (A-1) it has been assumed that the ideal gas equation of state can be applied to each of the species j comprising the gas mixture under consideration. This assumption is not strictly valid when the effect of screened Coulomb interactions is included and hence a different equation of state like that given in reference [8] could be more applicable.

It is equation (A-1) which is used in subroutine MAIN to find the chemical composition of an ionised gas. To account for screened Coulomb interactions using the Debye - Hückel approximation the chemical potential of each species j is modified to become:

$$\mu_j = \mu_j^0 + RT \ln (n_j/n) + RT \ln (P/101.3) - RTD_j \quad (A-3)$$

where the correction term D_j is represented by

$$D_j = - (eZ_j)^2 / (8\pi\epsilon_0 kT\rho_D) \quad (A-4)$$

and

$$\rho_D = (\epsilon_0 kT / \sum_j (eZ_j)^2 N_j)^{1/2} \quad (A-5)$$

In the above equations, ρ_D is the Debye radius, N_j is the number density of species j , Z_j is the charge number and ϵ_0 is the electrical permittivity of the vacuum.

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